Fluctuation Expansion in the Expected Value Evolution for Quantum Dynamics: Basic Issues and the Fluctuation Free Equations

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Abstract: In recent years, we have focused on the construction of ordinary differential equations (ODEs) for certain basic operators' expectation values whose totality suffice for describing the system's dynamics. This has been done for Quantum Dynamical Systems and the systems whose motion is governed by Liouville Equation. However, the starting point has been the construction of a linear set of ODEs for any given explicit ODE set even they are nonlinear in the description (right hand side) functions. The key idea was to use a complete basis set of unknown functions, each of which is functionally related at most to the unknown solution set of original ODEs. After some intermediate steps we could have been able to construct an infinite, first order, linear, homegeneous ODE set with a constant infinite square matrix coefficient. This infinite set of ODEs can be, in principal, analytically solved and the solution is unique as long as the initial conditions are given. The infinity could be handled by using appropriate truncation approximants in practical applications.

These equations define an evolution starting from a system state characterized by the initial vector which is a power vector whose block elements are the Kronecker powers of the system vector (which is composed of unknowns or the operators like momenta and positions in quantum mechanics) initial values. If the initial vector is not a power vector then there is a probabilistic nature in the initial vector because any vector can be expressed by the expectation values of the system vector's Kronecker powers with respect to a unique

weight function (see the moment problem). In these cases the probability distribution also evolves. Hence we have called the solution method to determine the motion defined by these equations "Probabilistic Evolution Approach (PEA)". Since the classical systems obey the causality, the probabilistic weight function in the initial vector and therefore in the solution for any time instance has to be exteremely sharp, zero-width-infinite-lenght, that is Dirac delta function.

This approach for ODEs has been quite appropriate to solve the equations of motion for classical dynamical systems. The quantum dynamical equivalent for the equations of motion for a given classical system is exactly same as the classical PEA in the infinite coefficient matrix if the mathmetical fluctuations are ignored. The only difference in the initial value vector. It is not a power vector. It is the expectation values of the Kronecker powers of the system vector under the probability density (the complex modulus square of the wave function). This brings the fluctuations (the differences between the expectation value of the system vector Kronecker power and the same power of the expectation value of the system vector) on the stage. Beyond that the fluctuations are not only on independent variables or their functions but operators bringing the noncommutative operator algeba to the method. These are just for initial values and the fluctuations for the infinite coefficient may change the face of the issue since quantum mechanics is governed by fluctuations as the considered system particle dimensions tends to diminish.

In this talk we use the one dimensional quantum systems for rather easy explanations even though the multidimensionality does not bring any noticeable complication except the increase in the number of routine manipulations. A rather general one dimensional quantum system can be defined via the following Hamilton operator.

$$\widehat{H} \equiv \frac{1}{2\mu}\widehat{p}^{\,2} + V\left(\widehat{q}\,\right) \tag{1}$$

where μ stands for the mass parameter while the definitions of the momentum $(\widehat{p}\,)$ and the position operator $(\widehat{q}\,)$ are given below

$$\widehat{p}f(x) \equiv -\hbar f'(x), \qquad \widehat{q}f(x) \equiv xf(x) \tag{2}$$

where $\hbar$ stands for the reduced Planck constant and x is called "position variable" which can take values from the real number set or its certain subdomain. The function $f(x)$ is assumed to be lying in the space where the wave function resides. It should be at least four times differentiable even though its analyticity preferable since otherwise the convergence issues may arise. The potential function is also preferably analytic even though second order differentiability suffices.

The starting formula to construct the fluctuation free approximation can be given as follows by skipping the derivation details in this extended abstract

$$\left\{\widehat{H}, \left\{\widehat{H}, f\left(\widehat{q}\right)\right\}\right\} = -\frac{1}{\mu} V'\left(\widehat{q}\right) f'\left(\widehat{q}\right) - \frac{2}{\mu} V\left(\widehat{q}\right) f''\left(\widehat{q}\right) + \frac{\hbar^2}{4\mu^2} f^{(4)}\left(\widehat{q}\right)$$
$$+ \frac{1}{\mu}\left[\widehat{H} f''\left(\widehat{q}\right) + f''\left(\widehat{q}\right)\widehat{H}\right] \qquad (3)$$

where the left hand side is autonomous as long as the Hamilton operator and the function f have no explicit time dependence. For this case we can write (3) as follows

$$\frac{d^2 \left\langle f\left(\widehat{q}\right)\right\rangle(t)}{dt^2} = -\frac{1}{\mu}\left\langle V'\left(\widehat{q}\right) f'\left(\widehat{q}\right)\right\rangle(t) - \frac{2}{\mu}\left\langle V\left(\widehat{q}\right) f''\left(\widehat{q}\right)\right\rangle(t) + \frac{\hbar^2}{4\mu^2}\left\langle f^{(4)}\left(\widehat{q}\right)\right\rangle(t)$$
$$\frac{2}{\mu} H_{exp}\left\langle f''\left(\widehat{q}\right)\right\rangle(t) + \frac{1}{\mu}\left\langle\left[\widehat{H}_f f''\left(\widehat{q}\right) + f''\left(\widehat{q}\right)\widehat{H}_f\right]\right\rangle(t) \qquad (4)$$

where $\widehat{H}_f \equiv \widehat{H} - H_{exp}\widehat{I}$ (where $\widehat{I}$ symbolizes the unit operator) defines the fluctuation in the Hamiltonian whose autonomous expectation value is denoted by the constant H_{exp}.

We call the cases where fluctuation containing terms are ignored, "Fluctuation free equation". By taking one of the elements of a basis set it is possible to construct sufficient number of equations to investigate the expectation value evolutions for the quantum system under consideration. The talk will focus on certain details of this issues.

Short Biography of Metin Demiralp

Metin Demiralp was born in Türkiye (Turkey) on 4 May 1948. His education from elementary school to university was entirely in Turkey. He got his BS, MS degrees and PhD from the same institution, İstanbul Technical University. He was originally chemical engineer, however, through theoretical chemistry, applied mathematics, and computational science years he was mostly working on methodology for computational sciences and he is continuing to do so. He has a group (Group for Science and Methods of Computing) in Informatics Institute of İstanbul Technical University (he is the founder of this institute).

He collaborated with the Prof. Herschel A. Rabitz's group at Princeton University (NJ, USA) at summer and winter semester breaks during the period 1985–2003 after his 14 month long postdoctoral visit to the same group in 1979–1980. He was also (and still is) in collaboration with a neuroscience group at the Psychology Department in the University of Michigan at Ann Arbour in last three years (with certain publications in journals and proceedings).

Metin Demiralp has more than 90 papers in well known and prestigious scientific journals, and, more than 200 contributions to the proceedings of various international conferences. He gave many invited talks in various prestigious scientific meetings and academic institutions. He has a good scientific reputation in his country and he was one of the principal members of Turkish Academy of Sciences since 1994. He has resigned on June 2012 because of the governmental decree changing the structure of the academy and putting politicial influence possibility by bringing a member assignation system. Metin Demiralp is also a member of European Mathematical Society. He has also two important awards of turkish scientific establishments.

The important recent foci in research areas of Metin Demiralp can be roughly listed as follows: Probabilistic Evolution Method in Explicit ODE Solutions and in Quantum and Liouville Mechanics, Fluctuation Expansions in Matrix Representations, High Dimensional Model Representations, Space Extension Methods, Data Processing via Multivariate Analytical Tools, Multivariate Numerical Integration via New Efficient Approaches, Matrix Decompositions, Multiway Array Decompositions, Enhanced Multivariate Product Representations, Quantum Optimal Control.